

PROCEEDINGS

Benchmarking Derivative-Free Optimization Strategies for Robust Crystal Plasticity Parameter Calibration

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ABSTRACT

Crystal plasticity (CP) models are powerful tools for describing the anisotropic deformation of metallic materials, yet their predictive capability hinges on accurate constitutive parameter calibration [1-3]. In practice, CP parameter identification is a computationally expensive inverse problem characterized by high-dimensional spaces, unavailable gradients, strong coupling, and significant prior uncertainty [4-7]. In this work, we formulate CP calibration as a budget-constrained black-box optimization problem and establish a unified benchmarking framework to systematically evaluate four representative derivative-free algorithms: Nelder-Mead (NM), Particle Swarm Optimization (PSO), Genetic Algorithm (GA), and Bayesian Optimization (BO). Three representative CP models—a BCC phenomenological model, an FCC dislocation-density model, and an HCP slip-twinning model—are investigated under narrow, medium, and wide prior domains. Our results demonstrate that BO exhibits the highest sample efficiency and robustness under wide priors, while GA provides the most stable surrogate-free baseline. In contrast, NM is competitive only in low-dimensional settings with restricted priors. Further analysis reveals that calibration difficulty is governed primarily by the parameter-error landscape structure rather than nominal dimensionality. Notably, we show that a low fitting error does not guarantee parameter identifiability due to substantial trade-offs among near-optimal combinations. This study provides practical guidance for selecting optimization strategies and offers insights into the robust calibration of advanced constitutive models.

KEYWORDS

Inverse modeling; ICME Strategies; surrogate-assisted optimization; budget-constrained optimization; constitutive behavior

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